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Two-Objective Solution Set Optimization to Maximize Hypervolume and Decision Space Diversity in Multiobjective Optimization

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***Abstract*—Diversity maintenance in the decision space is a recent hot topic in the field of evolutionary multiobjective optimization (EMO). In this paper, we propose the use of a decision space diversity measure as an objective function in a two-objective formulation of solution set optimization where the hypervolume measure is used as the other objective. In the proposed approach, a given multiobjective problem with an arbitrary number of objectives is handled as a two-objective solution set optimization problem. A solution of our two-objective problem is a set of non-dominated solutions of the original multiobjective problem. An EMO algorithm is used to search for a number of solution sets along the tradeoff surface between the diversity maximization in the decision space and the hypervolume maximization in the objective space. In this paper, first we numerically examine the diversity measure of Solow & Polasky (1994), which was used in recent studies of Ulrich et al. (2010, 2011), through computational experiments on many-objective distance minimization problems in a two-dimensional decision space. Then we formulate a two-objective solution set optimization problem to maximize the decision space diversity and the objective space hypervolume. Finally we demonstrate that a number of non-dominated solution sets can be obtained along the diversity-hypervolume tradeoff surface. Through computational experiments, we also examine the difference between the following two settings for diversity calculation: All solutions in a solution set are used in one setting while only non-dominated solutions are used in the other setting.**

Keywords-Evolutionary multiobjective optimization (EMO); decision space diversity; hypervolume; solution set optimization; indicator-based algorithms.

I. INTRODUCTION

Since early 1990s [1], [3], [4], [10], diversity maintenance has been an important research issue in the field of EMO (evolutionary multiobjective optimization) for the design of efficient EMO algorithms. The diversity of solutions has been discussed mainly in the objective space for multiobjective optimization whereas it has been discussed in the decision space for single-objective optimization [11]. This is because multiobjective optimization has been handled in the EMO community as the search for a solution set that approximates the entire Pareto front in the objective space very well. The Pareto front approximation is usually evaluated using the following two criteria: One is the proximity of solutions to the Pareto front, and the other is the diversity of solutions along the Pareto front. Both the proximity and the diversity are measured in the objective space.

Recently the importance of diversity maintenance in the decision space has been pointed out in the EMO community (e.g., see [13]). Test problems in a two-dimensional decision space have been also proposed to visually examine the decision space diversity of obtained solutions [7], [8]. When we discuss the diversity of solutions in the decision space, it is important to quantitatively measure the decision space diversity. Whereas some EMO algorithms such as Omni-Optimizer [6] have a decision space diversity maintenance mechanism, diversity measures in the decision space have not been actively studied in the EMO community. Recently, Ulrich et al. [14], [15] proposed the use of a diversity measure of Solow and Polasky [12] to evaluate the decision space diversity. It was shown in [14], [15] that the Solow-Polasky diversity measure has good theoretical properties.

Motivated by Ulrich et al. [14], [15], first we numerically examine the Solow-Polasky diversity measure [12] through computational experiments on many-objective test problems with a two-dimensional decision space [7], [8]. Then we formulate a two-objective solution set optimization problem to maximize the diversity of solutions in the decision space and the hypervolume in the objective space. Our approach can be classified as set-based multiobjective optimization [19]. One characteristic of our approach (and other approaches in set-based multiobjective optimization [19]) is that an individual is a set of solutions. Thus a population is a set of solution sets as in our former study [9] where a number of solution sets were obtained along the tradeoff surface between the hypervolume and the number of solutions. Another characteristic is to search for a number of solution sets along the tradeoff surface between the diversity of solutions in the decision space and the hypervolume in the objective space. Through computational experiments, we show that a large number of solution sets are obtained along such a tradeoff surface. We also demonstrate that totally different results are obtained from the following two settings with respect to diversity calculation: All solutions are used in one setting while only non-dominated solutions in each solution set are used in the other setting.

This paper is organized as follows. First we briefly explain the Solow-Polasky diversity measure [12] and its characteristic features [14], [15] in Section II. Next we examine whether the Solow-Polasky diversity measure coincides with our intuitive evaluation of the diversity through computational experiments on many-objective problems with a two-dimensional decision space in Section III. Then we formulate a two-objective solution set optimization problem to maximize the diversity in the decision space and the hypervolume in the objective space in Section IV. Experimental results are reported in Section V where NSGA-II is applied to the formulated two-objective problem. Finally we conclude this paper in Section VI.

II. SOLOW-POLASKY DIVERSITY MEASURE

Let us denote a set of n solutions $\{\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_n\}$ by P. Each solution $\boldsymbol{x}_i$ is a point in the decision space. We denote the distance between two solutions $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ by $d(\boldsymbol{x}_i, \boldsymbol{x}_j)$. The Euclidean distance is used to measure the distance. The Solow-Polasky diversity measure $D(P)$ is defined for the solution set P using the distance $d(\boldsymbol{x}_i, \boldsymbol{x}_j)$ as follows [12]:

$$D(P) = \mathbf{e}\mathbf{M}^{-1}\mathbf{e}^T , \quad (1)$$

where $\mathbf{e}$ is an n-dimensional vector of 1 (i.e., $\mathbf{e} = (1, 1, ..., 1)$) and $\mathbf{M}$ is an $n \times n$ matrix defined as

$$m_{ij} = \exp(-\theta \cdot d(\boldsymbol{x}_i, \boldsymbol{x}_j)) , \; i = 1,2, ..., n; \; j = 1,2, ..., n, \quad (2)$$

using a parameter θ. In our computational experiments, θ is specified as $\theta = 1$.

It was shown by Ulrich et al. [14], [15] that the diversity measure $D(P)$ has the following three properties:

(i) **Monotonicity in Varieties**: $D(P) < D(P \cup \boldsymbol{x})$ if $\boldsymbol{x} \notin P$. That is, when a new solution $\boldsymbol{x}$ is added to P, $D(P)$ increases. This property means that the addition of a new solution $\boldsymbol{x}$ always increases the diversity of a solution set P.

(ii) **Twinning**: $D(P) = D(P \cup \boldsymbol{x})$ if $\boldsymbol{x} \in P$. That is, when an existing solution $\boldsymbol{x}$ in P is added to P, $D(P)$ does not change. This property means that the addition of an existing solution $\boldsymbol{x}$ does not change the diversity of a solution set P.

(iii) **Monotonicity in Distance**: $D(P) \leq D(Q)$ if $d(\boldsymbol{x}_i, \boldsymbol{x}_j) \leq d(\boldsymbol{y}_i, \boldsymbol{y}_j)$ for all pairs of i and j where $P = \{\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_n\}$ and $Q = \{\boldsymbol{y}_1, \boldsymbol{y}_2, ..., \boldsymbol{y}_n\}$. This property means that the increase in the distance between solutions leads to the increase in the diversity.

III. NUMERICAL STUDY OF SOLOW-POLASKY MEASURE

In this section, we empirically examine whether the Solow-Polasky diversity measure $D(P)$ coincides with our intuitive evaluation of diversity through computational experiments. Whereas our examinations are totally subjective, we think that our observations will be acceptable for many researchers.

As a test problem, we use a five-objective minimization problem with a two-dimensional decision space $[0, 100] \times [0, 100]$ in our former study [8]. The five objectives are the distance to the five vertices of the regular pentagon in Fig. 1 (e.g., the first objective is the distance to the vertex A). All points inside the pentagon including its five sides are Pareto optimal solutions of this five-objective minimization problem.

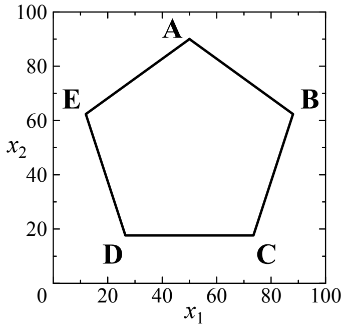

Figure 1. Our first test problem.

In our former study [8], we reported experimental results on this test problem by NSGA-II [5], SPEA2 [18], MOEA/D [17] and SMS-EMOA [2], [16]. In this paper, we also use Omni-Optimizer [6] with a decision space diversity maintenance mechanism. Moreover, we examine two different parameter specifications of the neighborhood size in MOEA/D: 1% and 10% of the population size (whereas the neighborhood size was specified as 10% of the population size in our former study [8]). In our preliminary computational experiments, we observed that the use of a small neighborhood structure had a positive effect on the diversity of solutions. Thus we examine the two specifications of the neighborhood size: 1% and 10%.

We performed our computational experiments in the same manner as in our former study [8]. That is, we used the following parameter specifications:

Coding: Real number strings of length 2,
Population size: 210 (in MOEA/D),
200 (in the other EMO algorithms),
Termination condition: 100,000 solution evaluations,
Crossover: SBX with $\eta_c = 15$,
Crossover probability: 1.0,
Mutation: Polynomial mutation with $\eta_m = 20$,
Mutation probability: 0.5,
Reference point:
Minimum value of each objective (in MOEA/D),
Maximum value of each objective $\times$ 1.1 (in SMS-EMOA).

Experimental results of a single run of each algorithm are shown in Fig. 2 where all solutions in the final population are depicted. The diversity measure $D(P)$ is calculated for each solution set (i.e., for all solutions depicted in each plot). The calculated value of the diversity measure is shown in the right-top corner of each plot. From the obtained solution sets in Fig. 2 (without looking at the calculated values of the diversity measure), we have the following observations:

(1) Fig. 2 (c) by SPEA2 seems to have the largest diversity.
(2) Fig. 2 (f) by SMS-EMOA seems to have the second largest diversity.
(3) Fig. 2 (b) by Omni-Optimizer seems to have a larger

diversity than Fig. 2 (a) by NSGA-II with no decision space diversity maintenance mechanism.

(4) Fig. 2 (d) by MOEA/D with the smaller neighborhood structure (MOEA/D (1%)) seems to have a larger diversity than Fig. 2 (e) by MOEA/D with the larger one.

The calculated values of the Solow-Polasky diversity measure in Fig. 2 coincide with the intuitive evaluation of the decision space diversity of each plot. One may feel that Fig. 2 (d) by MOEA/D (1%) has a larger diversity than Fig. 2 (a) by NSGA-II. This is true if we concentrate on solutions inside the pentagon. Due to the existence of many solutions outside the pentagon, Fig. 2 (a) has a larger diversity than Fig. 2 (d).

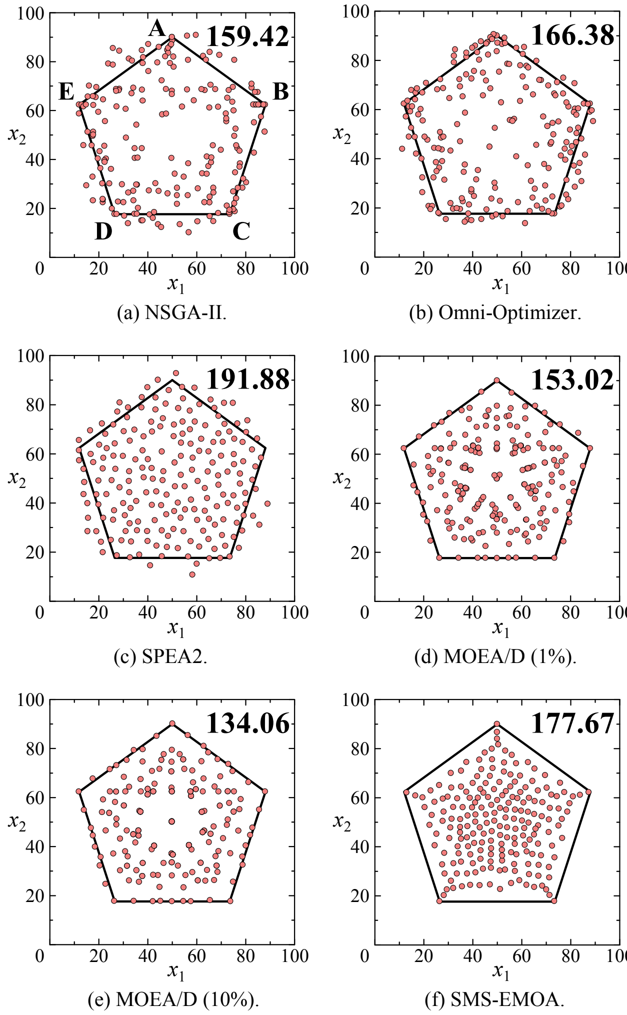

Figure 2. Experimental results of a single run of each algorithm on the first test problem.

Next we use a five-objective minimization problem in Fig. 3 with four copies of a regular pentagon. Each objective is the distance to the nearest vertex among the four vertices at the same position in each pentagon. For example, the first objective is the distance to the nearest vertex among A_1, A_2, A_3 and A_4 while the second objective is the distance to the nearest vertex among B_1, B_2, B_3 and B_4.

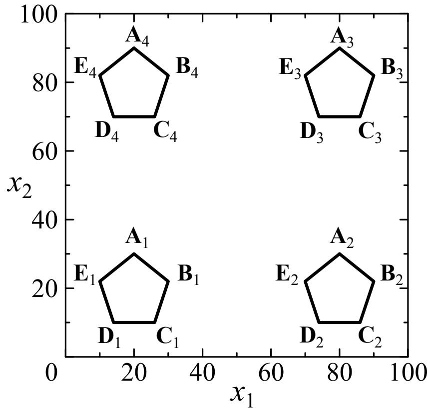

Figure 3. Our second test problem.

Experimental results are shown in Fig. 4 where we used the same parameter specifications as in Fig. 2. The used EMO algorithm is shown together with the calculated value of the diversity measure in each plot in Fig. 4.

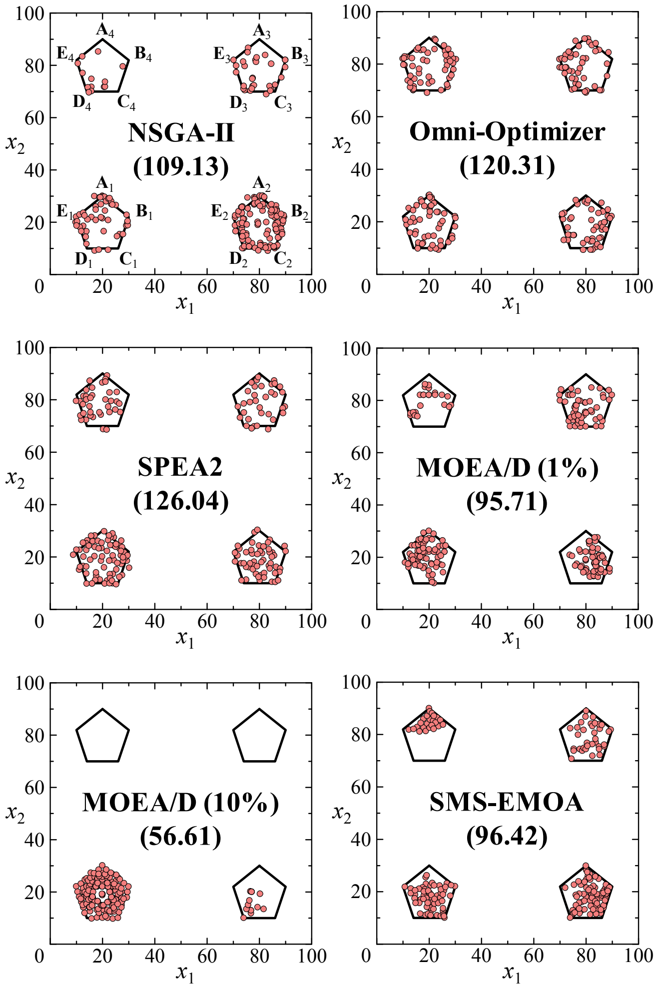

Figure 4. Experimental results of a single run of each algorithm on the second test problem.

From the distribution of obtained solutions in each plot (without looking at the calculated values of the diversity measure), we can obtain the following observations:

(1) The left-middle plot by SPEA2 and the right-top plot by Omni-Optimizer seem to have the largest diversity.
(2) The right-top plot by Omni-Optimizer seems to have a larger diversity than the left-top plot by NSGA-II.
(3) The left-bottom plot by MOEA/D (10%) with the large neighborhood structure seems to have the smallest diversity.

From Fig. 4, we can see that the calculated value of the diversity measure in each plot coincides with the intuitive evaluation of the diversity.

We also show our experimental results on a four-objective minimization problem in Fig. 5 [7]. This test problem was generated from the actual map. The four objectives are the distances to the nearest elementary school, junior high school, store and station (For details, see [7]). This problem has three Pareto optimal regions shaded in Fig. 5. One is the large shaded region with a complicated shape in the top-center. The other two Pareto optimal regions are very small (One is located south of the university, and the other is south of the top-left station).

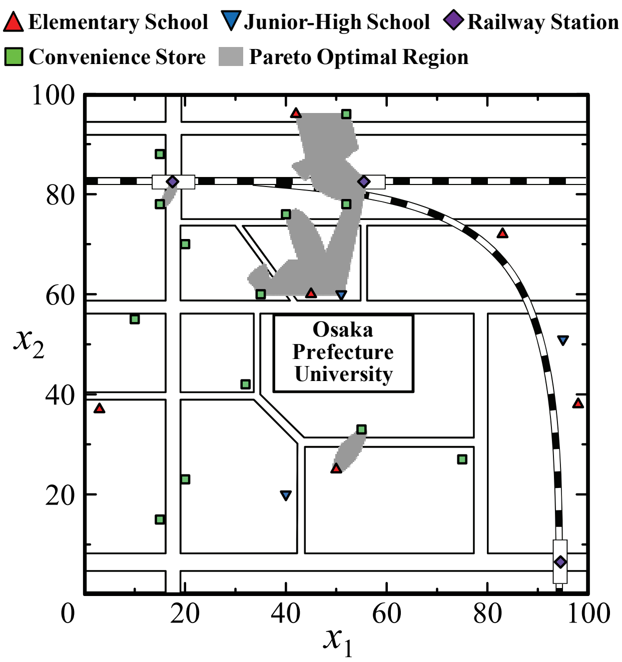

Figure 5. The third test problem generated from an actual map in our former study [7].

We used the same parameter specifications as in our former study [7], which are slightly different from the above-mentioned computational experiments (i.e., the computation load as the termination condition was increased from 100,000 to 200,000 solution evaluations, and the population size of MOEA/D was changed from 210 to 220). Experimental results are summarized in Fig. 6 (next page) where the used EMO algorithm and the calculated value of the diversity measure are shown at the top of each plot.

In Fig. 6, the left-middle plot by SPEA2 seems to have the largest decision space diversity among the six plots. Actually the largest value of the diversity measure is obtained from SPEA2 in Fig. 6. The right-top plot by Omni-Optimizer seems to have the second largest diversity. The second largest value of the diversity measure is obtained for the right-top plot.

IV. Two-Objective Solution Set Optimization

Let $H(P)$ be the hypervolume measure of a solution set P, which is calculated in the objective space. Using the hypervolume measure $H(P)$ in the objective space and the Solow-Polasky diversity measure $D(P)$ in the decision space, we formulate the following two-objective problem:

$$\text{Maximize } H(P) \text{ and } D(P) \text{ subject to } |P| = n, \qquad (3)$$

where n is the number of solutions in the solution set P, which is a pre-specified integer parameter. In this formulation, we implicitly assume that all solutions in P satisfy the constraint conditions of the original multiobjective problem.

The Solow-Polasky diversity measure $D(P)$ is calculated for all solutions in the solution set P. However, only non-dominated solutions in P are usually meaningful in the original multiobjective problem. Thus a variant of (3) can be formulated by using only non-dominated solutions in P in $D(P)$ as

$$\text{Maximize } H(P) \text{ and } D(ND(P)) \text{ subject to } |P| = n, \qquad (4)$$

where $ND(P)$ is the set of all non-dominated solutions in P.

V. Results of Two-Objective Set Optimization

We applied the two-objective set optimization problems in (3) and (4) to our second test problem in Fig. 3. First we uniformly discretized the two-dimensional decision space $[0, 100] \times [0, 100]$ into a 201×201 grid. This means that we only consider $201 \times 201 = 40401$ points as solutions of our test problem. Thus any solution set can be represented by a binary string of length 40401 where "1" in the binary string means the inclusion of the corresponding point. We used the NSGA-II with the following parameter specifications for the two-objective optimization problems in (3) and (4) with $n = 200$:

Coding: Binary strings of length 40401,
Population size: 200,
Termination condition: 400,000 solution evaluations,
Crossover: Uniform crossover,
Crossover probability: 0.8,
Mutation: Bit-flip mutation,
Mutation probability: 1/40401.

Since $n = 200$, the number of "1" in each string is always maintained as 200 by randomly adding "1" to each string (or removing "1" from each string) as needed after crossover and mutation. Experimental results of a single run of NSGA-II are shown in Fig. 7. Each solution in Fig. 7 (i.e., each open circle) is a solution set of our test problem. In Fig. 7, we have a large number of non-dominated solution sets along the hypervolume-diversity tradeoff surface.

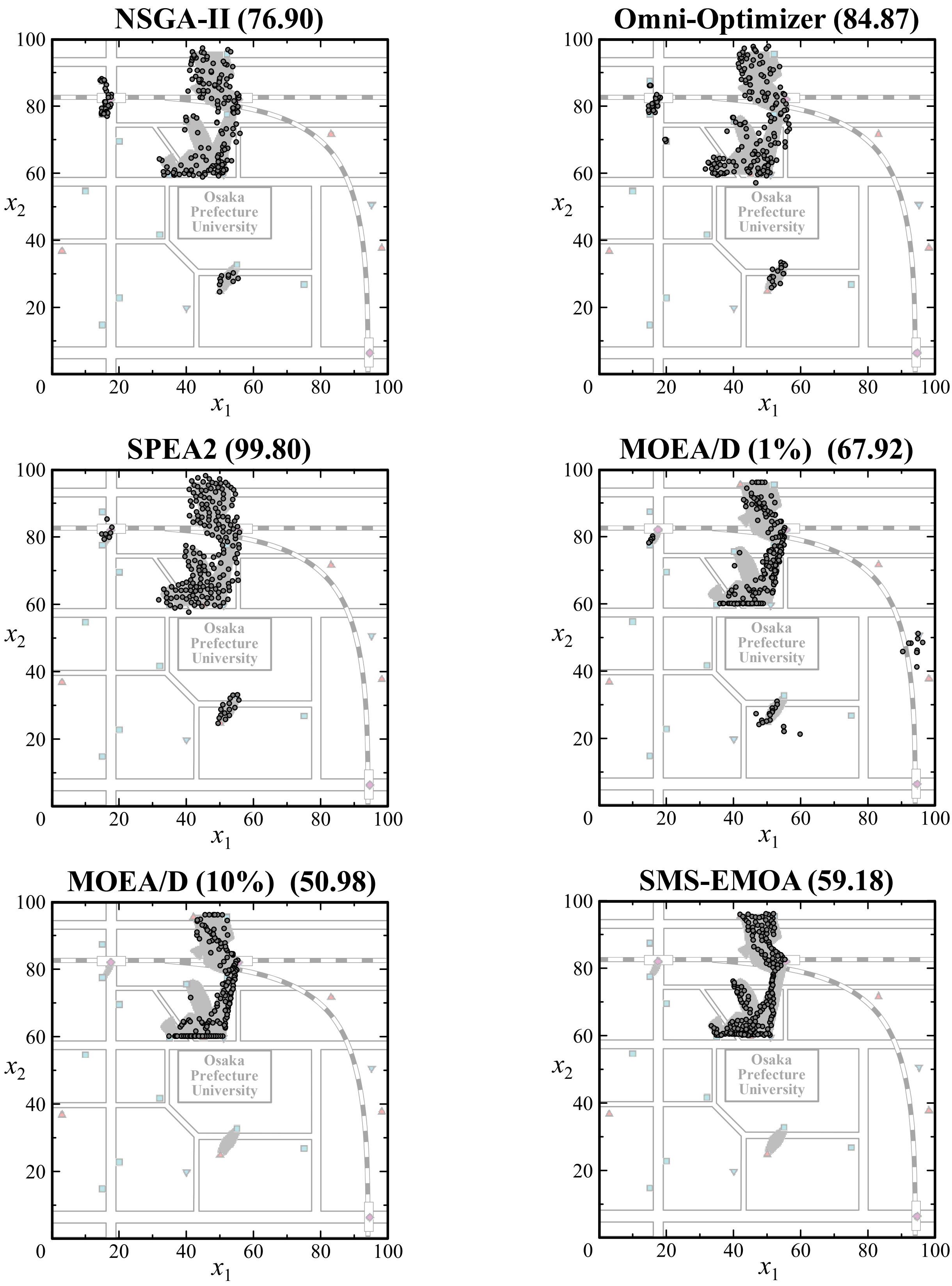

Figure 6. Experimental results of a single run of each algorithm on the third test problem.

Solution sets corresponding to A, B, C and D in Fig. 7 are shown in Fig. 8. From Fig. 8, we can see that totally different results were obtained from the two formulations: (3) and (4). When the diversity is calculated for all solutions (i.e., (3)), the diversity is maintained over the entire decision space as the solution sets A and B in Fig. 6. From the formulation in (4), good solution sets were obtained as shown by C and D in Fig. 8 (compare Fig. 8 with Fig. 4).

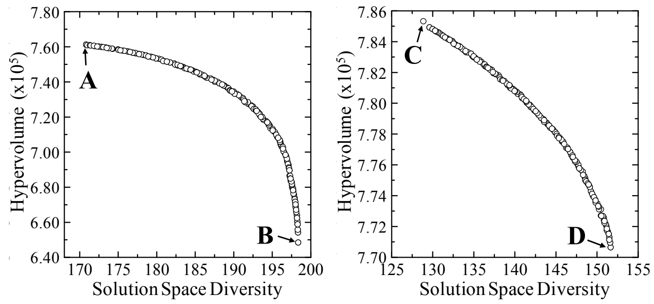

Figure 7. Results (Left: Formulation in (3), Right: Formulation in (4)).

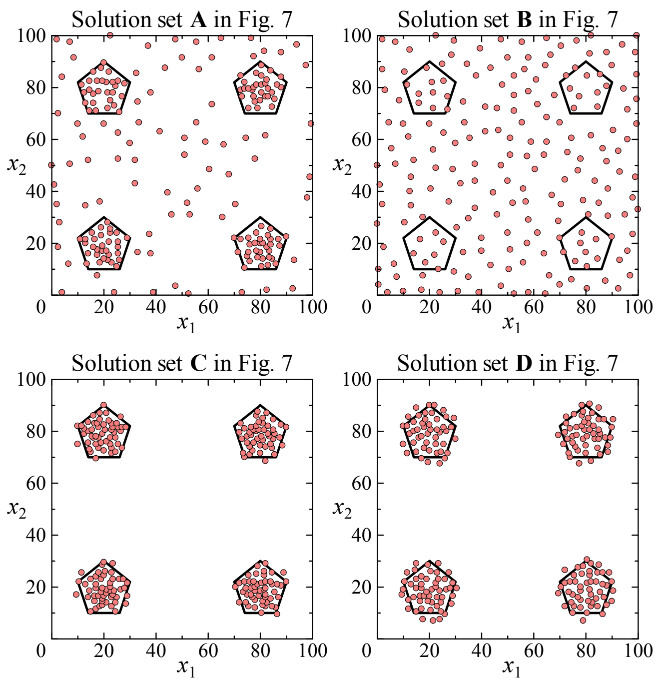

Figure 8. Solution sets corresponding to A, B, C and D in Fig. 7.

VI. CONCLUSIONS

We first demonstrated that the Solow-Polasky diversity measure [12] coincides with our intuition. This result will encourage further use of the diversity measure whereas our study was performed in a totally subjective manner. Then we formulated two-objective solution set optimization problems to simultaneously maximize the hypervolume and the Solow-Polasky diversity measure. Good solution sets were obtained when the diversity measure was calculated for non-dominated solutions in each solution set. When the diversity measure was calculated for all solutions, the diversity was maintained over the entire decision space. In this paper, we used a binary coding for the two-objective solution optimization problem. This is because we used a many-objective test problem with a two-dimensional decision space for enhancing visual explanation. A future research issue is applications of the proposed approach to more general multiobjective problems.

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